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TRANSFERABILITY OF A THREE-DIMENSIONAL AIR QUALITY MODEL BETWEEN TWO DIFFERENT SITES IN COMPLEX TERRAIN

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ABSTRACT

The three-dimensional, diagnostic, particle-in-cell transport and diffusion model MATHEW/ADPIC is used to test the transferability of this air quality model from one site in complex terrain to another with different characteristics, under stable night-time drainage flow conditions. The two sites were subject to extensive drainage flow tracer experiments under the multi-laboratory Atmospheric Studies in Complex Terrain (ASCOT) program: the first being a valley in the geothermal Geysers region of northern California, and the second a canyon in western Colorado. The domain in each case is approximately 10 x 10 km. Results from comparing computed with measured tracer concentrations indicate that 58% of the samples for Brush Creek and 51% for the Geysers agreed within a factor of 5. When an angular 10° uncertainty, consistent with anemometer reliability limits, was allowed to be applied to the model results, model performance improved such that 75% of samples compared within a factor of 2 for Brush Creek and 62% of samples within a factor of 2 for the Geysers. Results thus indicate that the model is satisfactorily transferable without tuning it to a specific site.

1. INTRODUCTION

The DOE (Department of Energy) ASCOT (Atmospheric Studies in Complex Terrain) program is designed to develop the technology needed to assess atmospheric properties and the impact of energy sources on air quality in regions of complex terrain, and to improve the fundamental knowledge of the physics of terrain dominated flows and of transport and diffusion processes. To this end the program relies heavily on development and validation of numerical models. The value of such models to a large part lies in their ability to reproduce results of equal quality when applied under a variety of conditions from siting studies to emergency response. Especially in the case of emergency response, when concentration data may be sparse initially, analysts must have a full degree of confidence in such a model.

One important step in developing confidence in a model is to test its transferability from one site to a different one under complex site conditions. In this connection, transferability is defined here as the capability of the model to give validation results of similar quality with the appropriate differences in input only, but without any tuning of it to any specific site. Chief factors affecting transferability are:

- Differences in topography and surface structure.
- Differences in the dominant flow characteristics of the site.
- Differences in the experimental design and methodology such as the layout of the meteorological and tracer instrumentation networks.
- Inadequacy of the model physics which may cause variable response to the complete physical picture.
- Numerical treatment of the validation process, such as grid resolution.

In this study, the three-dimensional, diagnostic, particle-in-cell transport and diffusion model MATHEW/ADPIC (M/A) is used to test the transferability of this air quality model from the ASCOT experimental site in the Geysers region of northern California to the Brush Creek site in western Colorado. The Geysers site is a bowl shaped valley and Brush Creek is a canyon with steep side walls. Both complex terrain sites were subject to extensive ASCOT tracer release campaigns: the Geysers in 1980 under nighttime drainage flow conditions and Brush Creek in 1984 under drainage flow and morning ventilation conditions. One night experiment was chosen for each site, that of September 20, 1980 in the Geysers and that of September 30, 1984 in Brush Creek. The experiments were different in many aspects of their meteorological conditions, duration, tracer release scenarios and meteorological instrumentation. These experiments were judged to be sufficiently rigorous to adequately test for model transferability.

This paper summarizes the M/A model, provides a description of the experiments and the method of evaluating the model transferability and, finally, presents and evaluates the results.

2. THE MATHEW/ADPIC (M/A) MODEL

The MATHEW model (Sherman, 1978) generates a mass conservative three-dimensional gridded mean wind field including terrain from available interpolated meteorological data and topography data bases. The input for the model consists of a digitized topographical surface, spacially interpolated surface winds and vertical wind profiles, and a stability parameter.

ADPIC (Lange, 1978 and 1981) is a three-dimensional, numerical diffusion and transport model capable of simulating the time and space varying dispersal of atmospheric pollutants under complex conditions. It is a particle-in-cell model in which Lagrangian "mass" particles are transported inside a fixed Eulerian grid. The model solves the three-dimensional diffusion-advection equation in flux conservative form,

$$\frac{\partial \chi}{\partial t} + \nabla \cdot \left(\chi \vec{U}_P \right) = 0 \qquad (1)$$

Here χ is the pollutant concentration and $\vec{U}_P$ is a pseudo velocity which is defined as the sum of the mean wind $\vec{U}_A$ and a diffusive velocity $\vec{U}_D$

$$\vec{U}_p = \vec{U}_A + \vec{U}_D; \quad \vec{U}_D \equiv -K \cdot \nabla\chi/\chi \qquad (2)$$

and K is the diffusivity parameter in the x, y, and z, directions. $\vec{U}_A$ is supplied by the MATHEW model.

ADPIC computes a horizontal and a vertical diffusivity K_h and K_z. K_h is based on the semi-empirical expression (Draxler, 1976)

$$\sigma_y = \sigma_\theta U t f\left(\frac{t}{\tau}\right); \quad f\left(\frac{t}{\tau}\right) = \left(1 + \frac{t}{\tau}\right)^{-1/2} \tag{3}$$

combined with the analytical relationship

$$K_h = \sigma_y d\sigma_y/dt \tag{4}$$

where σ_y is the horizontal standard deviation of the plume, σ_θ the standard deviation of the fluctuation of the wind direction, U the local mean wind speed, t is time, and $f(t/\tau)$ is a correlation function with an empirical time constant τ.

For the atmospheric surface layer K_z is based on similarity theory (Businger et al., 1971). In the outer atmospheric boundary layer K_z is of the form (Businger and Arya, 1974)

$$K_z = \frac{k u_* z}{\phi(z/L)} e^{-|V_g/u_*|z/h} \tag{5}$$

where k is the Von Karman constant, u_* is the friction velocity, z is the height above terrain, $\phi(z/L)$ is an atmospheric stability function based on z and the Monin-Obukhov scale length L, V_g is the geostrophic wind and h the height of the mixing layer. Both K_h and K_z (equations 4 and 5) are functions of x, y, z, and t.

The M/A model has been extensively evaluated with a number of experimental data sets with a wide variety terrain types, tracer release scenarios and meteorological conditions from INEL and SRP (Lange 1978), TMI (Dickerson et al. 1985), EPRI (Peterson and Lange 1984, Bowne and Bovenstein 1983), ASCOT (Lange and Myrup 1984), MATS (Rodriguez and Rosen 1984) Montalto (Desiato and Lange 1985) and Chernobyl (Lange et al. 1987). These studies have shown the M/A model capable of estimating air concentrations within a factor of two 50% of the time in flat or rolling terrain, while being within a factor of five 50% of the time in the cases of complex terrain and meteorology.

3. THE 1980 AND 1984 ASCOT EXPERIMENTS

A major common purpose in both the 1980 California Geysers and the 1984 Colorado Brush Creek experiments was to study nighttime drainage flow with the aid of inert, neutrally buoyant tracers. The terrain features, meteorological conditions and experimental layouts differed considerably for the two sites, and provide a good test for model transferability. The detailed descriptions of the experiments can be found in Gudiksen (1983) for the 1980 Geysers, and in Clements et al. (1987) for the 1984 Colorado Brush Creek campaign. For the purpose of this paper the description of the experiments will be largely limited to the stressing of their differences.

The Anderson Creek Valley in the Geysers area of northern California is a bowl shaped valley with mountains on the northeastern, northwestern and southwestern end and a ridge along the west with the only drainage opening to the southeast. It has rugged terrain and the ground cover ranges from bare soil to forest canopy. The change in elevation from the peak of the highest mountain in the northwest to the outflow in the east is about 1000 m. The area of interest for the experiment was about 12 x 9 km as indicated in the computer generated topography in Figure 1a. Also shown in this figure are the three drainage creeks designated as (A) for Anderson, (G) for Gunning and (P) for Putah Creek.

By contrast, the Brush Creek Canyon in western Colorado is a steep-walled, nearly straight V-shaped, 500 to 600 m deep canyon cut into a flat mesa. It runs from northwest to southeast where it opens into the larger Roan Creek Valley. It has a shallow drop of about 3° and 30–40° steep sidewalls and a number of smaller side canyons as shown in Figure 1b; also indicated are the Brush Creek (B) and Roan Creek (R). The domain of interest is roughly 11.5 x 12.5 km. The vegetation varies from bare rocks to tall shrubs.

The experiments chosen for this model transferability study are the drainage flow episodes of the night of September 19/20, 1980 from the Geysers and that of September 29/30, 1984 from Brush Creek. The extensive instrumentation that was deployed is shown in Table 1. The table shows that the Geysers experiment relied more on surface measurements with limited data taken to explore the vertical structure of the meteorology and the tracer distribution, while in Brush Creek heavy emphasis was laid on obtaining vertical profiles, especially of the tracer distribution. Additional differences in the experiments were the tracer releases. In the Geysers three one-hour surface releases of two perfluorocarbons and SF_6 took place from 2300 to 0000 PST, while in Brush Creek three perfluorocarbon tracers were released, one from the surface and one from 220 m within the canyon, and one from a side canyon near mesa height. The release duration was from 0000 to 0900 MST to catch the morning transition and canyon ventilation. As an example, Figure 2 shows the sampler layout for the two perfluorocarbons in the Geysers. Sampling times varied from 10 minutes to 2 hours. The release locations are indicated by the squares labeled PDCH and PMCH. In a similar fashion Figure 3 shows the sampler setup for Brush Creek. The heavy lines represent sampler arcs consisting of several samplers each. The squares are the release points and the triangles denote the many vertical tracer sampling locations.

Finally, the meteorology during the two experiments differed: while both sites displayed drainage flows along the creeks, the prevailing flow above the valley in the Geysers during the night of September 19/20, 1980 was a northwesterly sea breeze, almost aligned with the main drainage flow pattern. In contrast, on September 29/30, 1984 in Brush Creek the prevailing flow above the canyon top was from the southwest, almost at right angles to the north westerly drainage, causing strong directional shears at the transition level.

4. RESULTS AND DISCUSSION

A. Computations

The areas of interest and the size of the computational grid were very similar for the Geysers and for Brush Creek and roughly 10 x 10 km in scale. Grid resolution at 225 m per grid cell in the horizontal and 50 m (Geysers) and 40 m (Brush Creek) in the vertical was also comparable. Differences lay in the input and the time of the computer runs. The input differences, both for the meteorological and tracer parts, were discussed in the previous section. The running time for the Geysers M/A was six hours from 2300 PST September 19 to 0500 PST September 20, while the Brush Creek run was for 9 hours from 0000 MST to 0900 MST on September 30. Thus the Geysers run was strictly a drainage flow scenario while the Brush Creek run tried to capture also the early part of the morning flow reversal. The latter results must be viewed with great care because the ADPIC particle-in-cell model is unable to return particles once they have left the grid.

Figure 4 shows typical MATHEW windfields at 40 m above terrain. Figure 4a shows the winds at 9/20/0100 PST for the Geysers Anderson Valley. The convergence of the drainage winds towards the center of the bowl shaped valley and the outflow to the east are quite visible. The heavy dashed lines are the four main drainage creeks and the dot-dashed line indicates the mountain ridge line. The wind vectors are drawn at every other grid point. Corresponding wind fields for Brush Creek are shown in Figure 4b and 4c. Figure 4b shows a well organized drainage flow down-canyon at 0100 MST, while Figure 4c shows the somewhat disorderly return flow at 0900 MST. The flow vectors on the mesas are questionable because no wind measurements were taken there to guide the MATHEW model.

Typical examples of the particle plumes representing the tracer releases are shown in Figure 5. Significant differences can be observed between the Geysers Anderson Valley plume in Figure 5a and the Brush Creek plume in Figure 5b. The Geysers Anderson Creek surface release plume is shown at 0100 PST one hour after the end of the release and is fairly short and disorganized having more of a shape between a plume and a puff. In contrast, the Brush Creek surface release plume shown at 0300 MST is well behaved and well organized because of the confines of the steep side walls of the canyon.

B. Quantitative Analysis of Transferability

Before giving statistical results of the approximately 1000 samples taken to judge model transferability, some comparisons typical for the types of individual concentration sampling techniques are illustrated. The Geysers M/A evaluation studies have been extensively covered in Lange (1984, 1985) and emphasis will be given here to Brush Creek comparisons.

In both experiments time of arrival of the plume was measured by sequential samplers at several distances from the source. Figure 6 shows the measured and computed concentrations at the surface for sequential sampler BS1, located near the mouth of Brush Creek some 8 km from the source, as a function of time for the surface release. The results for time of arrival and concentrations are quite good, and starting at 0800 MST the effect of the creek ventilation due to heating is visible both in the measurements and the M/A values. Results for the Geysers were of similar quality at the sequential samplers.

Two examples of the vertical profiling of the tracer from the surface release in Brush Creek are shown in Figures 7 and 8. Figure 7 shows the concentrations as a function of height for two time periods 0200–0300 MST and for 0700–0800 MST, at the PNL profiler near the mouth of the creek valley 8 km from the release point. Figure 8 shows similar information at the LLNL site about 5 miles from the release point. Measurements and M/A results compare quite well on the whole but there is a tendency for M/A to overpredict at the mid level heights and underpredict at the surface. This may be caused by the shape of the vertical diffusivity function (equation 5 in Section 2) which is strictly valid only for flat terrain. It was pointed out that vertical profiling of the tracers at the Geysers was sparse, but essentially displayed the same effect as observed in Brush Creek: despite nighttime stable drainage flow conditions, the surface release tracers were measured up to 400 m in the vertical only some 8 km from the source.

In terms of M/A modeling of both sites, the vertical diffusion coefficients had to be raised by the equivalent of at least one Pasquill category over stable conditions. The reason for this is probably the shear interaction of various small drainage flow contributions into the main flow at different heights and temperatures. An additional feature seen in Figure 8b is the onset of the Brush Creek ventilation. In the Geysers increased horizontal diffusion was required by M/A to simulate meandering. Because of the confinement of the steep Brush Creek canyon sidewalls no quantitative comparison could be made, however, both sites were modeled with the same, increased horizontal eddy diffusivities.

It is difficult to devise a statistical process that adequately describes a model's performance when compared to tracer field data, particularly when the field data span a broad spectrum of release and sampling times, sampling distances, terrain and meteorology. The standard correlation coefficient is used sometimes; however, one point at the high end of the scale can influence the entire data set. These points in the Geysers and in Brush Creek are typically located close-in to the tracer release point where high concentrations are present, and the plumes are narrow so that spatial resolution is critical. Here, and especially in complex terrain, a difference of 2 to 5° in the angle of the computed plume trajectory can produce outlying points that completely overshadow the performance of the model in the rest of the domain under study.

In addition, clusters of samplers deployed to provide an estimate of the spatial variability of measurements in complex terrain have differed by factors of 3 to 5 in concentrations in some cases. Figure 9 illustrates this point with samplers BS1 and B29. Figure 9 shows the rectified sampler arc 1 with sampler numbers and relative locations versus surface concentrations about 8 km from the release point. (The longest heavy Cross Canyon line in Figure 3). Within the figure a scale indicates the length equivalent to an angle of 10° at the source. It can be seen that an angular deviation of the computed from the actual tracer plume of less than 5° greatly reduces agreement.

In order to test the transferability of M/A between the Geysers and Brush Creek a method was chosen that is less easily biased by a few high concentrations. It is a band analysis which equally weights the model performance over the entire spatial domain of interest by using the ratio of measured over computed tracer concentration samples within the grid volume. A factor R is computed for each pair of measurements (C_m) and model calculations (C_c) which represents the whole-number ratio between the two. The percent of comparisons within a factor R are plotted as a function of R. The definition of R is $R = (C_m + B)/(C_c + B)$, except if $R < 1$, then $R = (C_c + B)/(C_m + B)$, and B is background which is added to C_m if appropriate. If both C_m and C_c are zero, the sample is disregarded.

In addition, in order to provide computed sample concentrations with a range of error bars, an area of uncertainty A is drawn around a sampler location. The size of the area A is defined in terms of an angle of uncertainty $\pm\delta\theta$ as shown in Figure 10. For each sampler, the distance r between the source S and the location of the sampler M is determined, and for a given angular uncertainty $\pm\delta\theta$ the area of computational uncertainty is $A = (2r\delta\theta)^2$. The computed maximum and minimum concentrations C_{c+} and C_{c-} within this area A are determined and are considered the upper and lower extent of an error bar associated with the computed sampler concentration C_c.

If, for any given sampler, the measured concentration C_m lies within this error bar, i.e. $C_{c+} \geq C_m \geq C_{c-}$, the computed concentration C_c is considered to be the same as mesured C_m in the evaluation of the model. For any postulated angular error $\delta\theta$, the R factor analysis can be performed such that,

$$\begin{aligned} \text{if } C_m \geq C_{c+} \quad \text{then R} &= (C_m + B)/(C_{c+} + B), \\ \text{if } C_{c+} \geq C_m \geq C_{c-} \quad \text{then R} &= 1, \\ \text{if } C_m \leq C_{c-} \quad \text{then R} &= (C_{c-} + B)/(C_m + B). \end{aligned} \tag{6}$$

In the case of $\delta\theta = 0$ this scheme reduces to the conventional R factor analysis described above.

Figure 11 shows the results of the M/A transferability evaluation between the Geysers and Brush Creek sites. The curves represent the percentage of samples for which measurements compare with computed values of tracer concentrations to within the factor R defined above. The solid lines represent the Geysers, and the dashed lines the Brush Creek M/A validation. Also, the curves with solid symbols (circles and triangles) represent exact comparison in space and time, ($\delta\theta = 0$), while the curves with open symbols allow for an angular uncertainty of $\delta\theta = \pm\ 5°$. This size of uncertainty was chosen because it roughly corresponds to the error of anemometer readings for wind direction.

In terms of transferability of M/A from the Geysers to Brush Creek, Figure 11 shows that the model results are quite similar for each site, despite the differences of topography and the design of the tracer experiments. M/A did slightly better for Brush Creek probably because of the more orderly air flow due to the confinement of the canyon walls. Otherwise the curves indicate the same improvement of results with increasing R. Of special interest is the striking improvement of the model performance when it is allowed an angular uncertainty equivalent to that for measurements.

The figure also shows the total number of samples to be roughly the same, and the average measured and computed values and the residuals indicate that M/A underestimated the concentrations in the Geysers and overestimated in Brush Creek. This is largely due to how well M/A can model close-in tracer samples of high concentrations, given the complex topography and wind structure. Since nothing but the M/A input parameters were different for the two sites i.e. no site specific tuning of the model was done, it can be said that the model successfully transferred from the Geysers to Brush Creek.

5. SUMMARY AND CONCLUSIONS

The ASCOT tracer release experiments of the night of September 20, 1980 in the Geysers of Northern California, and of the night of September 30, 1984 in Brush Creek in western Colorado, were used to determine if the three-dimensional, diagnostic, particle-in-cell transport and diffusion model MATHEW/ADPIC is transferable between these two different sites and experiments. Transferability here is defined as the model giving validation results of similar quality with the appropriate differences in input only but without any tuning of the model to any specific site.

The sites differed considerably in terrain—the Geysers a bowl shaped valley, and Brush Creek a canyon with steep walls. In addition, the experiments differed considerably in their meteorological conditions, duration, tracer release times and duration, and in the design of the meteorological and tracer network and methodology.

In order to avoid the dominance over the results by close-in samples with high concentrations, which typically are hard to match in complex terrain, a band analysis was chosen which weights each sample equally within the entire domain of interest (model grid). In this analysis the percentage of measured samples that agree with those computed within a factor R are determined. In this comparison 58% of the samples for Brush Creek and 51% for the Geysers agreed within a factor of 5—a typical ratio for complex terrain. Other ratios (Figure 11) support the result that the model was transferable with confidence. When an angular $\pm\ 5^{\circ}$ uncertainty (error bar), consistent with anemometer reliability limits, was allowed to be applied to the model results, model performance increased dramatically by the same measure for both Brush Creek (75% of samples within a factor of 2) and the Geysers (62% of samples within a factor of 2).

6. ACKNOWLEDGMENTS

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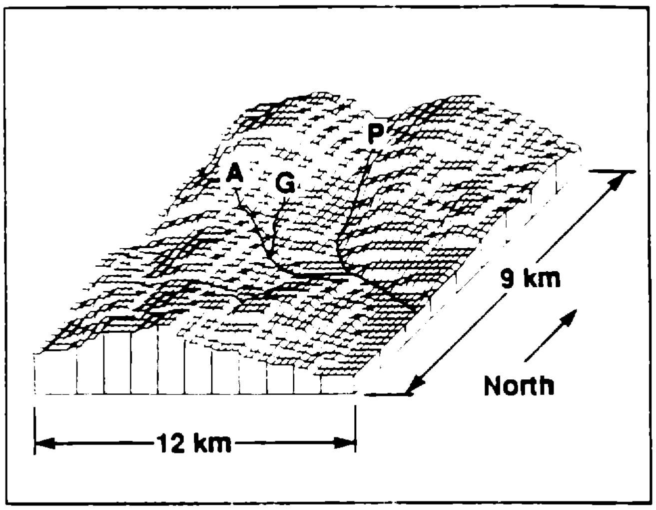
Table 1. Instrumentation of the ASCOT 1980 and 1984 field studies.

Instrument	Number	
	1984	1980
Tethersonde	11	7
Doppler Acoustic Sounder	7	1
Vertical Turbulence Profiler	1	-
Instrumented Towers	19*	39
Optical Anemometer Paths	13	8
Surface Energy Budget Stations	5	-
Doppler Lidar	1	-
Upper Air Stations	5	2
Tracers (Perfluorocarbons and SF_6)	3	3
Vertical Tracer Profilers	10	2
Surface Tracer Samplers	90	84

*In the main flow of the canyon.

(a)



(b)

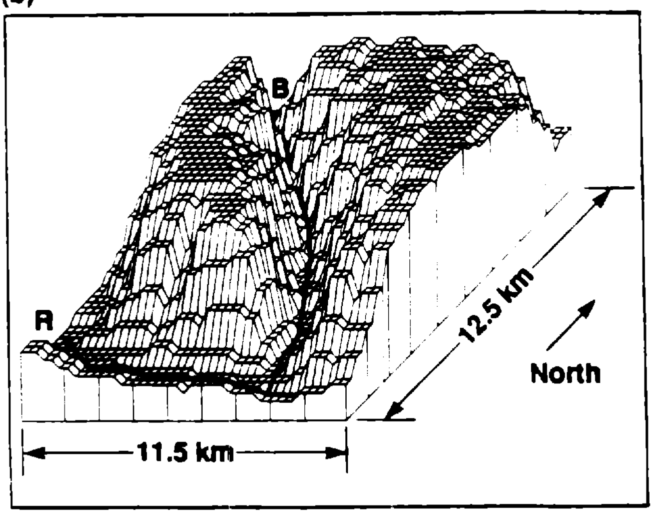


Figure 1. Computer generated topography of (a) the Anderson Creek Valley in the Geysers and (b) the Brush Creek canyon. The drainage creeks are indicated by the dark lines.

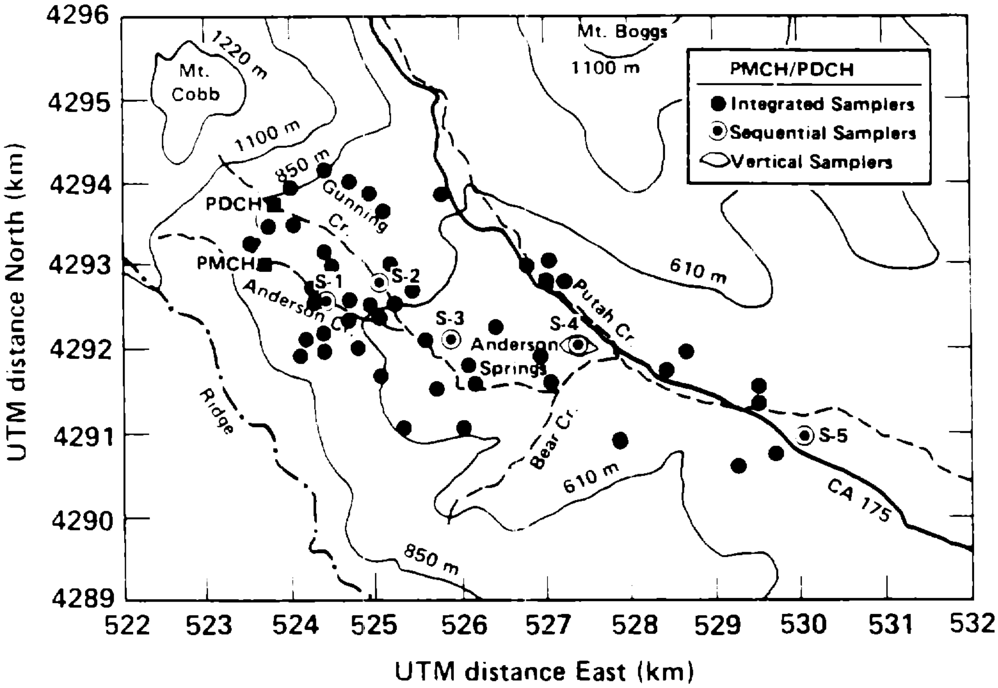


Figure 2. Sampling and release locations for the two perfluorocarbons at the 1980 Geysers Anderson Creek valley experiments. The squares labeled PMCH and PDCH designate the release points.

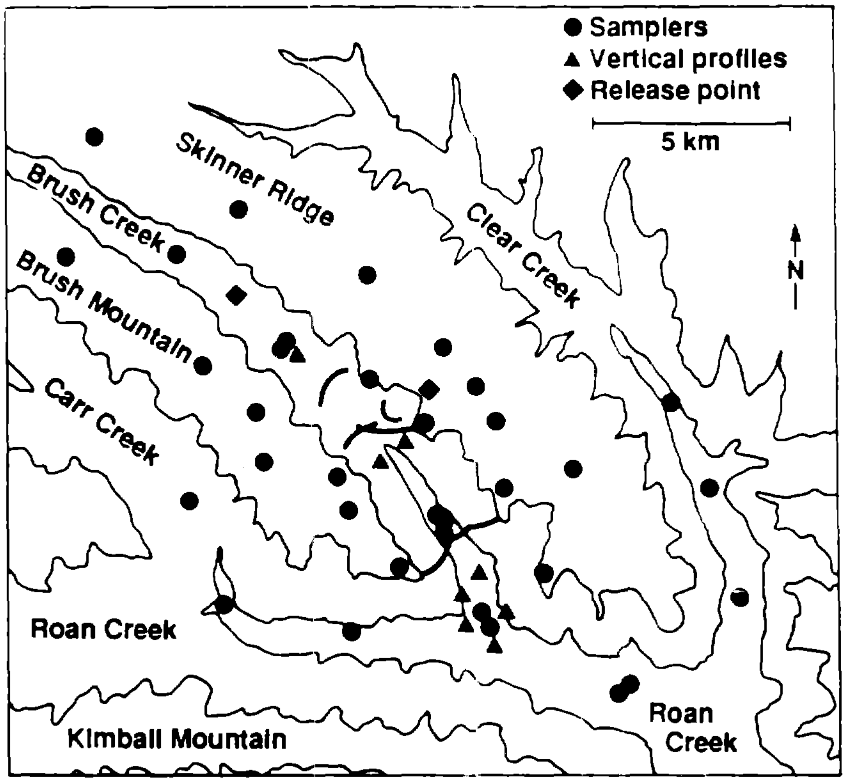


Figure 3. Sampling and release locations for the 1984 Brush Creek tracer experiments. The heavy solid lines are sampler arcs each consisting of several samplers.

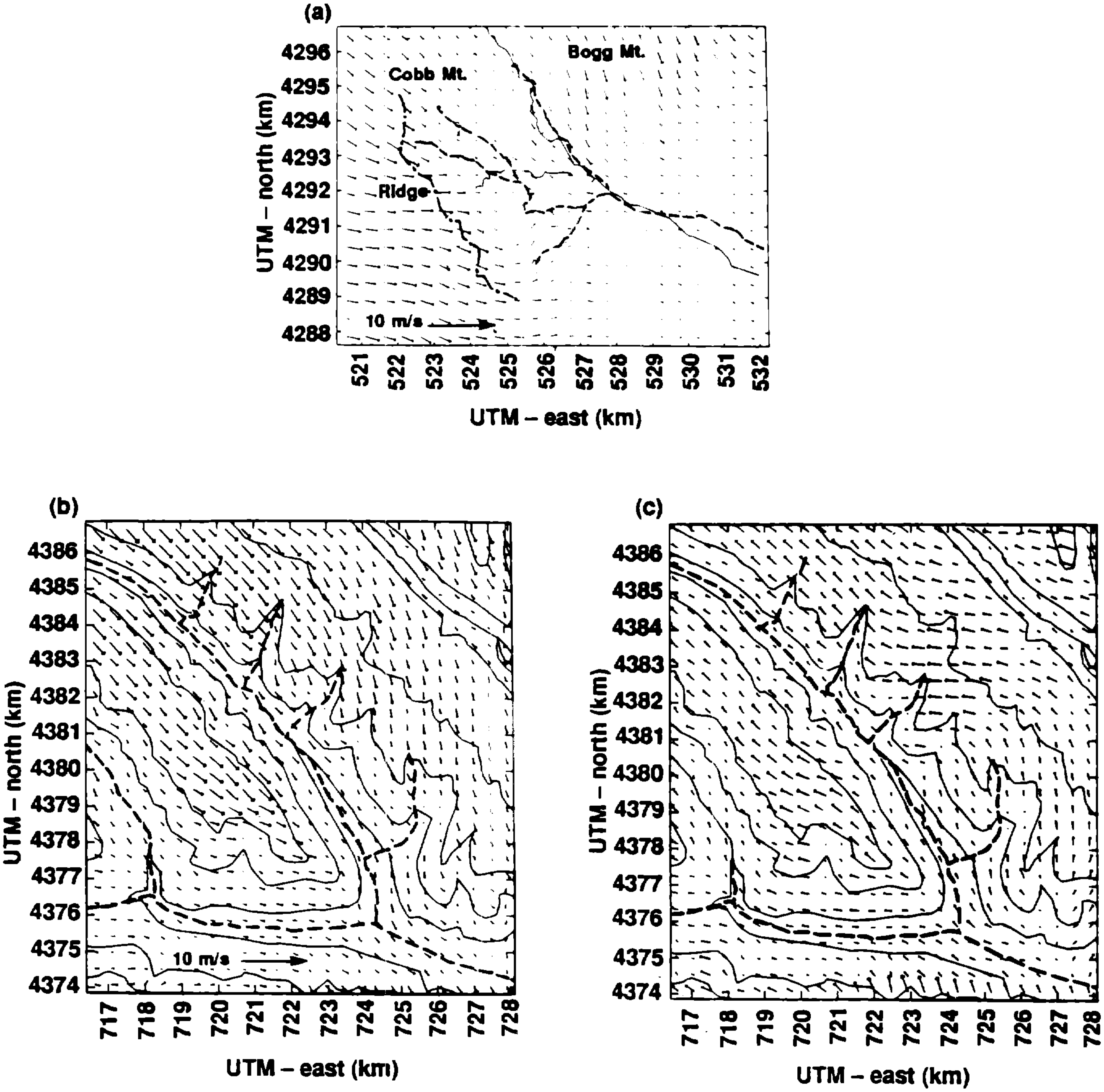


Figure 4. Examples of the windfields at 40 m above terrain. (a) for the drainage episode of the September 19/20, 1980 Geysers experiment at 0100 PST. (b) the night of the September 29/30, 1984 Brush Creek experiment, at 0100 MST during drainage and (c) at 0900 MST during flow reversal. Dashed lines are the creeks.

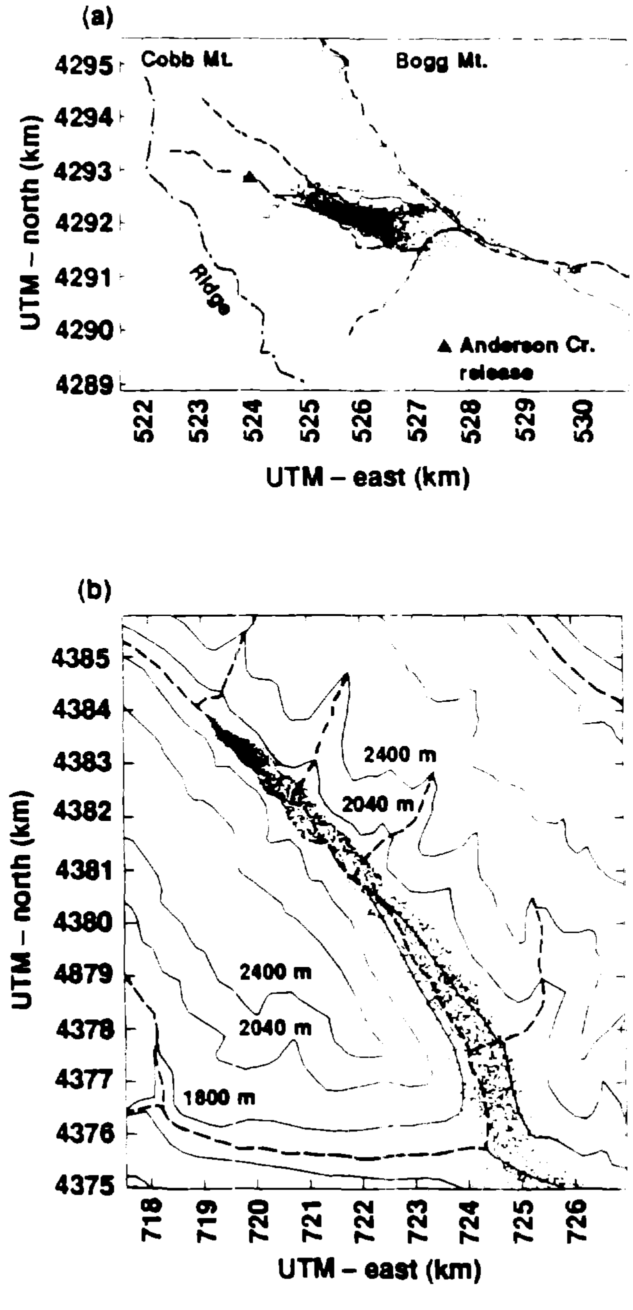


Figure 5. ADPIC plume simulations. (a) is an example of a particle plume representing one of the perfluorocarbon releases in the Geysers Anderson valley at 0100 PST one hour after the end of the release. (b) is a similar depiction of the Brush Creek surface release at 0300 MST. The heavy dashed lines are the creeks.

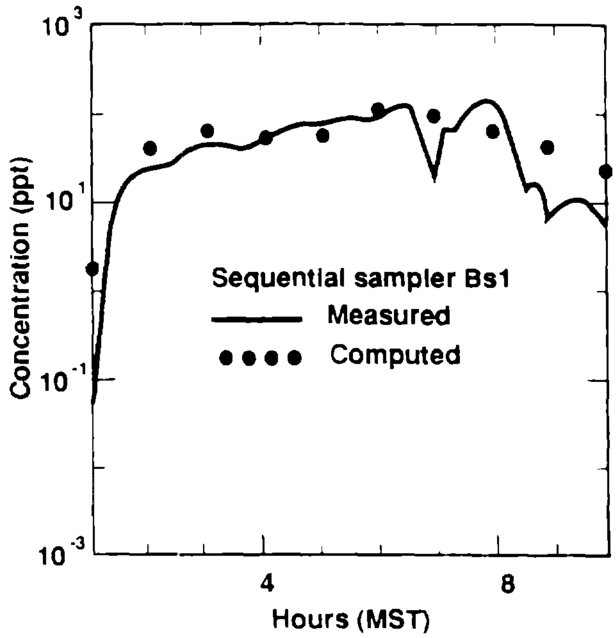


Figure 6. Measured and computed concentrations from the Brush Creek surface release as a function of time at the sequential sampler BS1 some 8 km from the source.

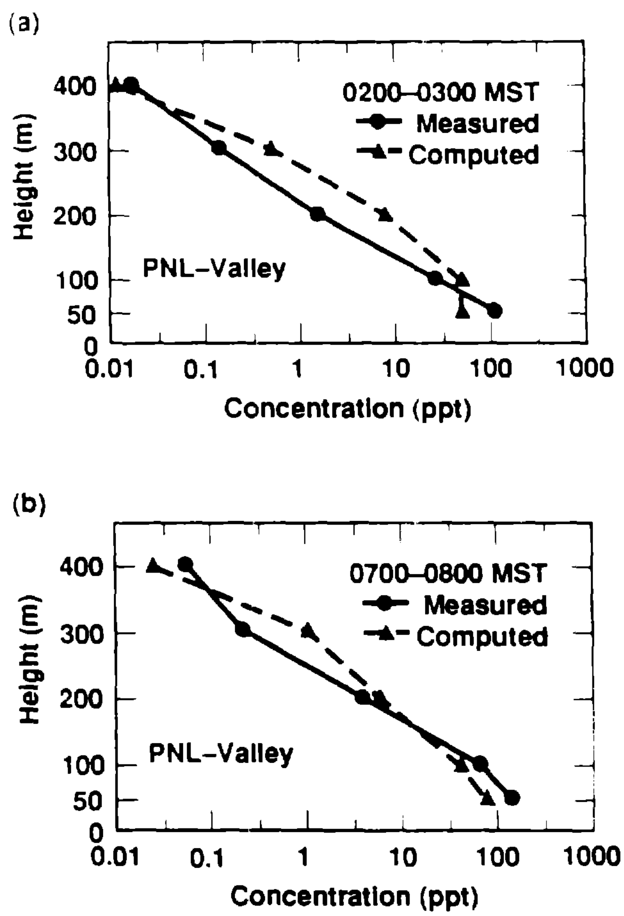


Figure 7. Measured and computed tracer concentrations as a function of height at the PNL profiler near the Brush Creek valley mouth, some 8 km from the surface source on 9/30/84. (a) 0200–0300 MST, (b) 0700-0800 MST.

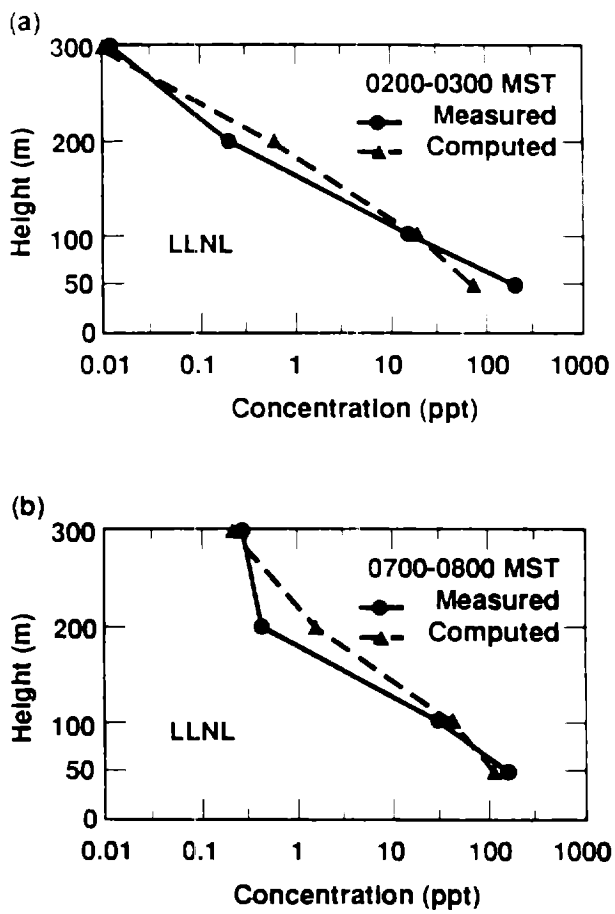


Figure 8. Same as Figure 7 except for the LLNL profile station some 5 km from the source.

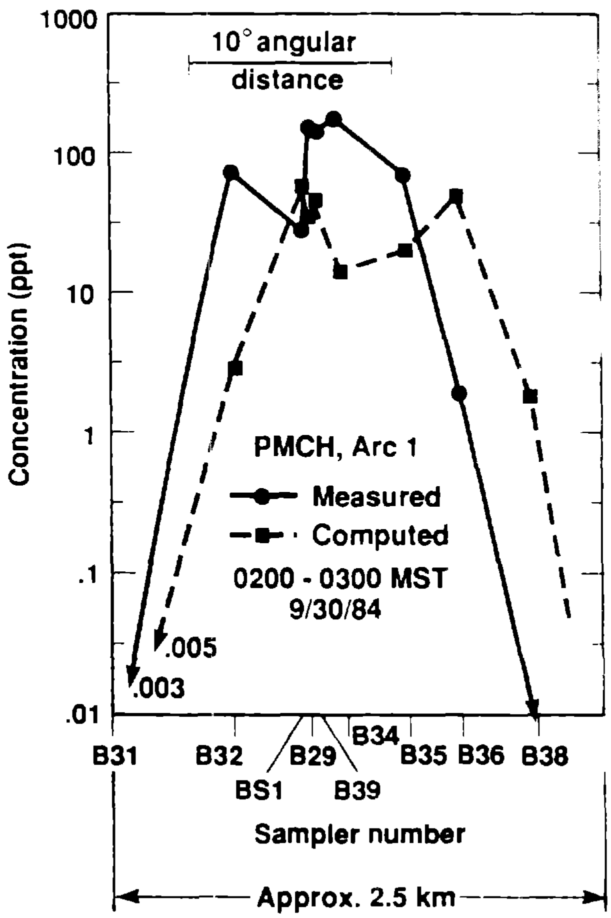


Figure 9. Surface tracer plume concentrations versus sampler location along the sampler arc 1 about 8 km from the release point for the Brush Creek surface release. The scale within the figure denotes a 10° difference in angle of the plume trajectory.

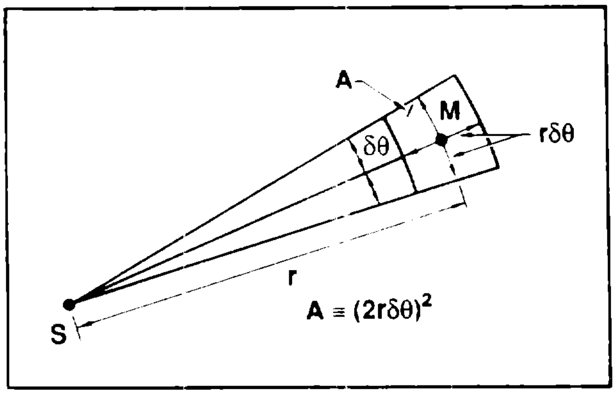


Figure 10. Area of uncertainty A, defined by the angular uncertainty $\pm\delta\theta$. M is the location of the sampler and r is the distance of the sampler from the source S.

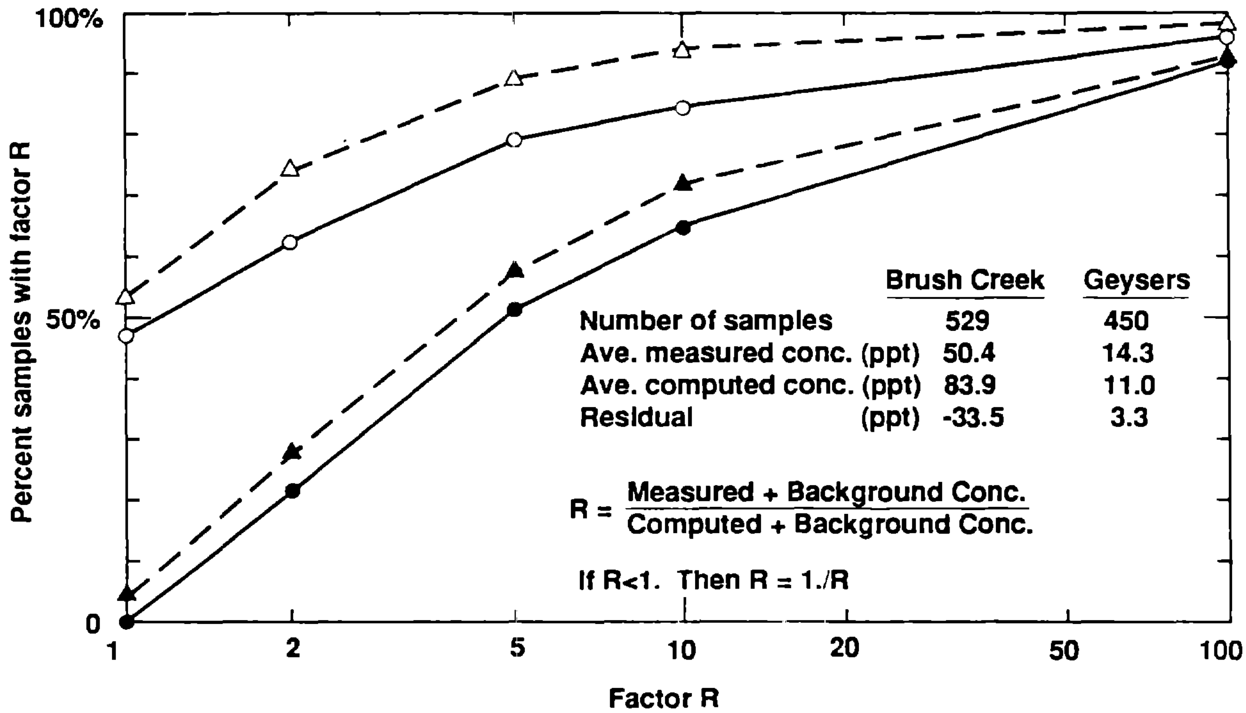


Figure 11. Percentage of measured samples agreeing with those computed to within a factor R as defined in the figure. Solid lines are for the 1980 Geysers, dashed lines for the 1984 Brush Creek simulations. The solid circles and triangles indicate exact comparison in space and time while the open symbols indicate curves showing results allowing a $\pm$ 5° error in the model calculations. Simulations are for the 9/20/80 Geysers and the 9/30/84 Brush Creek experiments.